

Quantum cascade laser simulation using an sp^3s^* full Brillouin zone tight-binding model

Jeremy Green, Corrie Farmer, Michel Garcia, Hock Koon Lee, Colin Stanley and Charles Ironside
University of Glasgow, Electronics and Electrical Engineering Department, Oakfield Avenue, Glasgow, G12 8LT, UK

Gerhard Klimeck
Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Drive, MS 169-315 Pasadena, CA 91109-8099, U.S.A.

Roger Lake
Department of Electrical Engineering, University of California, Riverside, CA 92521-0425, U.S.A.

The quantum cascade laser (QCL) is an electrically pumped unipolar semiconductor laser based on intersubband transitions in quantum wells. It is capable of coherent light emission over a wavelength range of at least $3.5\text{ }\mu\text{m}$ to $88\text{ }\mu\text{m}$, and its main application is as a light source for optical gas sensors. The gain medium of a QCL is composed typically of 25 to 35 identical stages, each containing perhaps 16 epitaxial layers. Given the resulting large number of design parameters, a tool that can accurately model the properties of the gain medium is required to optimise the device performance and to tailor the emission wavelength.

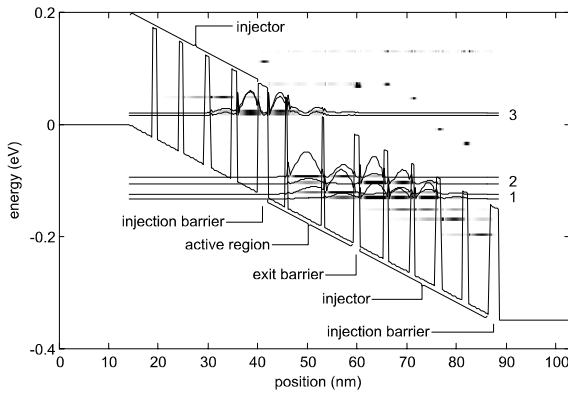


FIG. 1. The resonant states found for the AlAs/GaAs design of Becker *et al.* [2]. The moduli squared of the sums of the tight-binding expansion coefficients for each lattice plane are shown for all the resonant states using grey scale bars and in addition, for the pairs of states forming levels 1, 2 and 3, with curves. The bulk conduction band edge energy is also plotted: for the AlAs barriers, this is the bulk X-valley energy.

The first steps towards producing such a tool are reported here. The NanoElectronic MOdeling 3.0.2 software package [1], *NEMO*, has been used to calculate the electronic structure of a portion of various

biased QCL gain media. The second nearest neighbour sp^3s^* tight-binding model used is capable of accurately modelling the conduction band non-parabolicity and the X-like nature of some of the resonances. The results of such a calculation for a particular AlAs/GaAs QCL gain medium are shown in fig. 1.

The electronic structure of various other QCL gain medium designs have been simulated and the results used to make predictions of the photon energy at which the gain coefficient is maximized (E_{peak}). These predictions have been compared with experimental data for the same designs – see fig 2.

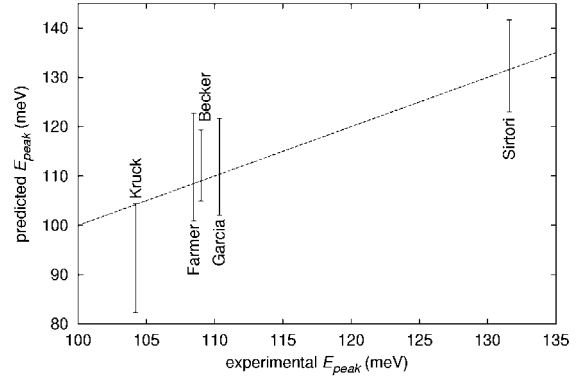


FIG. 2. Comparison of predicted and experimental photon energies that maximize the gain coefficient for various QCL gain medium designs. The straight line shows the ideal case of perfect agreement between the predictions and the experimental results.

The results from the tight-binding model calculations have also been compared to results from empirical two-band $k\cdot p$ model simulations. It has been shown that the tight-binding model is better able to predict E_{peak} and is able to model states with X-like character.

[1] <http://www-hpc.jpl.nasa.gov/PEP/gecko/nemo>

[2] Cyrille Becker, Carlo Sirtori, Hideaki Page, Geneviève Glastre, Valentin Ortiz, Xavier Marcadet, Max Stellmacher and Julien Nagle. AlAs/GaAs quantum cascade lasers based on large direct conduction band discontinuity. *Appl. Phys. Lett.* **77**, 463 (2000).